

Characterization of majorization monotone quantum dynamics

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Abstract—In this article I study the dynamics of open quantum system in Markovian environment. I give necessary and sufficient conditions for such dynamics to be majorization monotone, which are those dynamics always mixing the states.

I. INTRODUCTION

In the last two decades, control theory has been applied to an increasingly wide number of problems in physics and chemistry whose dynamics are governed by the time-dependent Schrödinger equation (TDSE), including control of chemical reactions [1], [2], [3], [4], [5], [6], [7], [8], state-to-state population transfer [9], [10], [11], [12], [13], shaped wavepackets [14], NMR spin dynamics [15], [16], [17], [18], [19], Bose-Einstein condensation [20], [21], [22], quantum computing [23], [24], [25], [26], [27], oriented rotational wavepackets [28], [29], [30], etc. More recently, there has been vigorous effort in studying the control of open quantum systems which are governed by Lindblad equations, where the central object is the density matrix, rather than the wave function [31], [32], [33], [34], [35], [36], [37]. The Lindblad equation is an extension of the TDSE that allows for the inclusion of dissipative processes. In this article, I will study those dynamics governed by Lindblad equations and give necessary and sufficient conditions for the dynamics to be majorization monotone, which are those dynamics always mixing the states. This study suggests that majorization may serve as time arrow under these dynamics in analog to entropy in second law of thermal dynamics.

The article is organized as following: section II gives a brief introduction to majorization; section III gives the definition of majorization monotone quantum dynamics; then in section IV, necessary and sufficient conditions for majorization monotone quantum dynamics are given.

II. BRIEF INTRODUCTION TO MAJORIZATION

In this section I give a brief introduction on majorization, most stuff in this section can be found in the second chapter of Bhatia's book [42].

For a vector $x = (x_1, \dots, x_n)^T$ in \mathbb{R}^n , we denote by $x^\downarrow = (x_1^\downarrow, \dots, x_n^\downarrow)^T$ a permutation of x so that $x_i^\downarrow \geq x_j^\downarrow$ if $i < j$, where $1 \leq i, j \leq n$.

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Definition 1 (majorization) A vector $x \in \mathbb{R}^n$ is majorized by a vector $y \in \mathbb{R}^n$ (denoted by $x \prec y$), if

$$\sum_{j=1}^d x_j^\downarrow \leq \sum_{j=1}^d y_j^\downarrow \quad (1)$$

for $d = 1, \dots, n-1$, and the inequality holds with equality when $d = n$.

Proposition 1 $x \prec y$ iff x lies in the convex hull of all $P_i y$, where P_i are permutation matrices.

Proposition 2 $x \prec y$ if and only if $x = Dy$ where D is doubly stochastic matrix.

Remark 1 A doubly stochastic matrix D is a matrix with non-negative entries and every column and row sum to 1, i.e., $d_{ij} \geq 0$, $\sum_i d_{ij} = 1$, $\sum_j d_{ij} = 1$.

Proposition 3 Suppose f is a convex function on \mathbb{R} , and $x \prec y$ in \mathbb{R}^n , then

$$\sum_i^n f(x_i) \leq \sum_i^n f(y_i).$$

Proposition 4 For a vector $\lambda = (\lambda_1, \dots, \lambda_n)^T$, denote D_λ a diagonal matrix with $(\lambda_1, \dots, \lambda_n)$ as its diagonal entries, let $a = (a_1, \dots, a_n)^T$ be the diagonal entries of matrix $A = K^T D_\lambda K$, where $K \in SO(n)$. Then $a \prec \lambda$. Conversely for any vector $a \prec \lambda$, there exists a $K \in SO(n)$, such that $(a_1, \dots, a_n)^T$ are the diagonal entries of $A = K^T D_\lambda K$.

Remark 2 $SO(n)$ is the group of special orthogonal matrices, $K \in SO(n)$ means $K^T K = I$ and $\det(K) = 1$.

III. MAJORIZATION IN OPEN QUANTUM DYNAMICS

The state of an open quantum system of N -level can be represented by a $N \times N$ positive semi-definite, trace 1 matrix, called density matrix. Let ρ denote the density matrix of an quantum system, its dynamics in markovian environment is governed by the Lindblad equation, which takes the form

$$\dot{\rho} = -i[H(t), \rho] + L(\rho), \quad (2)$$

where $-i[H, \rho]$ is the unitary evolution of the quantum system and $L(\rho)$ is the dissipative part of the evolution. The term $L(\rho)$ is linear in ρ and is given by the Lindblad form [38], [40],

$$L(\rho) = \sum_{\alpha\beta} a_{\alpha\beta} (F_\alpha \rho F_\beta^\dagger - \frac{1}{2} \{F_\beta^\dagger F_\alpha, \rho\}),$$

where F_α, F_β are the Lindblad operators, which form a basis of $N \times N$ trace 0 matrices (we have $N^2 - 1$ of them) and $\{A, B\} = AB + BA$. If we put the coefficient $a_{\alpha\beta}$ into a $(N^2 - 1) \times (N^2 - 1)$ matrix $A = (a_{\alpha\beta})$, it is known as the GKS (Gorini, Kossakowski and Sudarshan) matrix [39], which needs to be positive semi-definite.

Eq. (2) has the following three well known properties: 1) $\text{Tr}(\rho)$ remains unity for all time, 2) ρ remains a Hermitian matrix, and 3) ρ stays positive semi-definite, i.e. that ρ never develops non-negative eigenvalues.

Definition 2 Suppose ρ_1 and ρ_2 are two states of a quantum system, we say ρ_1 is majorized by ρ_2 ($\rho_1 \prec \rho_2$) if the eigenvalues of ρ_1 is majorized by the eigenvalues of ρ_2 ($\lambda(\rho_1) \prec \lambda(\rho_2)$).

Basically majorization gives an order of mixed-ness of quantum states, i.e., if $\rho_1 \prec \rho_2$, then ρ_1 is more mixed than ρ_2 , which can be seen from the following propositions.

Definition 3 (Von Neumann entropy) The Von Neumann entropy of a density matrix is given by

$$S(\rho) = -\text{Tr}[\rho \log(\rho)].$$

Proposition 5 If $\rho_1 \prec \rho_2$, then $S(\rho_1) \geq S(\rho_2)$.

Proposition 6 If $\rho_1 \prec \rho_2$, then $\text{Tr}(\rho_1^2) \leq \text{Tr}(\rho_2^2)$.

Remark 3 The above two propositions can be easily derived from Proposition 3.

The entropy and trace norm are usually used to quantify how mixed quantum states are. But majorization is a more strong condition than these two functions, and in some sense it gives a more proper order of mixed-ness as we can see from the following proposition.

Proposition 7 [44] $\rho_1 \prec \rho_2$ if and only if ρ_1 can be obtained by mixing the unitary conjugations of ρ_2 , i.e., $\rho_1 = \sum_i p_i U_i \rho_2 U_i^\dagger$, where $p_i > 0$, $\sum_i p_i = 1$ and U_i are unitary operators.

IV. NECESSARY AND SUFFICIENT CONDITION OF MAJORIZATION MONOTONE QUANTUM DYNAMICS

Definition 4 (Majorization monotone dynamics) An open quantum dynamics governed by Eq. (2) is majorization monotone if and only if $\rho(t_2) \prec \rho(t_1)$ when $t_2 > t_1$, $\forall t_1, t_2$.

Intuitively majorization monotone dynamics are those kind of dynamics which always mixing the states. As we can see from Proposition 5, these kind of dynamics always increase the entropy of the system. One can immediately see a necessary condition for a dynamics to be majorization monotone: the state $\rho_I = \frac{1}{N}I$ has to be a steady state of such dynamics, where I is identity matrix. As $\frac{1}{N}I$ is the most mixed state,

any state $\rho_i \prec \frac{1}{N}I$ would imply $\rho_i = \frac{1}{N}I$. The question now is whether this condition is also sufficient.

Let's first look at a simple system: a single spin in markovian environment.

A. An example on single spin

Take the general expression of the master equation

$$\dot{\rho} = -i[H, \rho] + L(\rho), \quad (3)$$

where

$$L(\rho) = \sum_{\alpha\beta} a_{\alpha\beta} (F_\alpha \rho F_\beta^\dagger - \frac{1}{2} \{F_\beta^\dagger F_\alpha, \rho\}).$$

For the single spin, we can take the basis $\{F_\alpha\}$ as normalized Pauli spin operators $\frac{1}{\sqrt{2}}\{\sigma_x, \sigma_y, \sigma_z\}$, where $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, and $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. The coefficient matrix

$$A = \begin{pmatrix} a_{xx} & a_{xy} & a_{xz} \\ a_{yx} & a_{yy} & a_{yz} \\ a_{zx} & a_{zy} & a_{zz} \end{pmatrix}$$

is positive semi-definite.

If identity state is a steady state, the right hand side of Eq. (3) should be 0 when $\rho = \frac{1}{N}I$. As $-i[H, \frac{1}{N}I] = 0$, so the condition reduces to $L(I) = 0$ (since $L(\rho)$ is a linear map, we can ignore the constant $\frac{1}{N}$). This is equivalent to

$$\sum_{\alpha,\beta} a_{\alpha\beta} [F_\alpha, F_\beta^\dagger] = 0. \quad (4)$$

In the single spin case, substitute F by Pauli matrices and it is easy to see that the above condition reduces to

$$a_{\alpha\beta} = a_{\beta\alpha},$$

i.e., the GKS matrix should be real symmetric, positive semi-definite matrix [41], while the general GKS matrix is Hermitian, positive semi-definite. We want to see whether the dynamics of single spin under this condition is majorization monotone.

As majorization monotone is defined by the eigenvalues of density matrices, we are going to focus on the dynamics of the eigenvalues of density matrix. Let Λ be its associated diagonal form of eigenvalues of density matrix ρ , i.e., Λ is a diagonal matrix with eigenvalues of ρ as its diagonal entries. At each instant of time, we can diagonalize the density matrix $\rho(t) = U(t)\Lambda(t)U^\dagger(t)$ by a unitary matrix $U(t)$.

Substitute $\rho(t) = U(t)\Lambda(t)U^\dagger(t)$ into Eq. (2), we get

$$\begin{aligned} \dot{\rho}(t) &= \dot{U}(t)\Lambda(t)U^\dagger(t) + U(t)\dot{\Lambda}(t)U^\dagger(t) \\ &\quad + U(t)\Lambda(t)\dot{U}^\dagger(t) \\ &= -iH'(t)U(t)\Lambda(t)U^\dagger(t) + U(t)\dot{\Lambda}(t)U^\dagger(t) \\ &\quad + U(t)\Lambda(t)U^\dagger(t)iH'(t) \\ &= -i[H'(t), U(t)\Lambda(t)U^\dagger(t)] + U(t)\dot{\Lambda}(t)U^\dagger(t) \\ &= -i[H(t), U(t)\Lambda(t)U^\dagger(t)] + L[U(t)\Lambda(t)U^\dagger(t)], \end{aligned} \quad (5)$$

where $H'(t)$ is defined by $\dot{U}(t) = -iH'(t)U(t)$, which is Hermitian. We obtain

$$\begin{aligned}\dot{\Lambda}(t) &= U^\dagger(t) \{-i[H(t) - H'(t), U(t)\Lambda(t)U^\dagger(t)] \\ &\quad + L[U(t)\Lambda(t)U^\dagger(t)]\} U(t) \\ &= -i[U^\dagger(t)(H(t) - H'(t))U(t), \Lambda(t)] \\ &\quad + U^\dagger(t)L[U(t)\Lambda(t)U^\dagger(t)]U(t).\end{aligned}\quad (6)$$

Note that the left side of the above equation is a diagonal matrix, so for the right side we only need to keep the diagonal part. It is easy to see that the diagonal part is zero for the first term, thus we get

$$\dot{\Lambda}(t) = \text{diag}(U^\dagger(t)L[U(t)\Lambda(t)U^\dagger(t)]U(t)), \quad (7)$$

where we use $\text{diag}(M)$ to denote a diagonal matrix whose diagonal entries are the same as matrix M .

$$\begin{aligned}\dot{\Lambda}(t) &= \text{diag}(U^\dagger L(U\Lambda U^\dagger)U) \\ &= \text{diag}\left(\sum_{\alpha\beta} a_{\alpha\beta} (U^\dagger F_\alpha U \Lambda U^\dagger F_\beta^\dagger U \right. \\ &\quad \left. - \frac{1}{2} \{U^\dagger F_\beta^\dagger U U^\dagger F_\alpha U, \Lambda\})\right) \\ &= \text{diag}\left(\sum_{\alpha\beta} a_{\alpha\beta} (U^\dagger F_\alpha U \Lambda U^\dagger F_\beta U \right. \\ &\quad \left. - \frac{1}{2} \{U^\dagger F_\beta U U^\dagger F_\alpha U, \Lambda\})\right).\end{aligned}\quad (8)$$

For the last step we just used the fact that F_β is a Pauli matrix which is Hermitian. Now

$$U^\dagger F_\alpha U = c_{\alpha\gamma} F_\gamma,$$

where $C = \begin{pmatrix} c_{xx} & c_{xy} & c_{xz} \\ c_{yx} & c_{yy} & c_{yz} \\ c_{zx} & c_{zy} & c_{zz} \end{pmatrix} \in SO(3)$ is the adjoint representation of U . Substituting these expressions into Eq. (8), we obtain

$$\dot{\Lambda}(t) = \text{diag}\left(\sum_{\alpha\beta} a'_{\alpha\beta} (F_\alpha \Lambda F_\beta - \frac{1}{2} \{F_\beta F_\alpha, \Lambda\})\right), \quad (9)$$

where

$$a'_{\alpha\beta} = c_{\gamma\alpha} a_{\gamma\mu} c_{\mu\beta}$$

are entries of transformed GKS matrix,

$$A' = C^T A C.$$

We can write $\Lambda(t) = \begin{pmatrix} \frac{1}{2} + \lambda(t) & 0 \\ 0 & \frac{1}{2} - \lambda(t) \end{pmatrix} = \frac{1}{2}I + \lambda(t)\sigma_z$, where $\lambda(t) \in [0, \frac{1}{2}]$. Substitute it into Eq. (9), we obtain the dynamics for $\lambda(t)$,

$$\dot{\lambda}(t) = -(a'_{11} + a'_{22})\lambda(t).$$

From Proposition 4, we know

$$\mu_3 + \mu_2 \leq a'_{11} + a'_{22} \leq \mu_2 + \mu_1,$$

where $\mu_1 \geq \mu_2 \geq \mu_3$ are eigenvalues of the GKS matrix. From this it is easy to see that at time T , the value of $\lambda(T)$ lies in the following interval

$$[e^{-(\mu_1 + \mu_2)T}\lambda(0), e^{-(\mu_2 + \mu_3)T}\lambda(0)],$$

which is always less or equal to $\lambda(0)$. And this is sufficient for the dynamics to be majorization monotone in the single spin case, as $(\frac{1}{2} + \lambda(T), \frac{1}{2} - \lambda(T)) \prec (\frac{1}{2} + \lambda(0), \frac{1}{2} - \lambda(0))$ when $\lambda(T) \leq \lambda(0)$. So $L(I) = 0$ is necessary and sufficient for the dynamics to be majorization monotone in the single spin case. And this condition holds even we have coherent control on the spin, as the identity state remains as steady state in the presence of control as we can see from the following controlled dynamics:

$$\dot{\rho} = -i[H(t) + \sum_i u_i H_i, \rho] + L(\rho),$$

where $\sum_i u_i H_i$ are our coherent controls. Suppose the controllers are able to generate any unitary operations on the spin fast compare to the dissipative rate, then $\lambda(T)$ can actually take any value in the interval $[e^{-(\mu_1 + \mu_2)T}\lambda(0), e^{-(\mu_2 + \mu_3)T}\lambda(0)]$, i.e., the reachable set for the single spin under the controlled Lindblad dynamics is

$$\begin{aligned}\rho(T) &= \{U \begin{pmatrix} \frac{1}{2} + \lambda(T) & 0 \\ 0 & \frac{1}{2} - \lambda(T) \end{pmatrix} U^\dagger | \lambda(T) \in \\ &\quad [e^{-(\mu_1 + \mu_2)T}\lambda(0), e^{-(\mu_2 + \mu_3)T}\lambda(0)], U \in SU(2)\}.\end{aligned}$$

This is to say that although controls can't reverse the direction of mixing, it can change the rate within some region.

Remark 4 From the single spin case, we can see that a dynamical system being majorization monotone does not imply the states of the system always converge to identity state, as identity being a steady state does not exclude the possible existence of other steady states, for example, the dynamics given by

$$\dot{\rho} = -i[\sigma_z, \rho] + \gamma[\sigma_z, [\sigma_z, \rho]],$$

which describes the transverse relaxation mechanism in NMR, satisfies the majorization monotone condition in the single spin case, and it is easy to see that the state of this system does not necessary converge to identity matrix, in fact it can well be converged to any state of the form $\frac{1}{2}I + \alpha\sigma_z$, where $\alpha \in [0, \frac{1}{2}]$.

B. General Case

In this section, we will show that $L(I) = 0$ is also sufficient for the dynamics to be majorization monotone in the general case. Suppose we solved the Lindblad equation

$$\dot{\rho} = -i[H(t), \rho] + L(\rho), \quad (10)$$

integrated this equation from t_1 to t_2 , where $t_2 > t_1$, and get a map:

$$\Psi : \rho(t_1) \rightarrow \rho(t_2).$$

Such a map has a Kraus operator sum representation [40], [43]:

$$\rho(t_2) = \Psi(\rho(t_1)) = \sum_i K_i \rho(t_1) K_i^\dagger, \quad (11)$$

where in our case $\{K_i\}$ are $N \times N$ matrices, which depend on the dynamical Eq. (10) and the time difference between t_1

and t_2 . Also the Kraus operator sum has to be trace preserving as the trace of density matrix is always 1, which implies that

$$\sum_i K_i^\dagger K_i = I.$$

If we have additional condition that identity state is a steady state of this dynamics, which means if $\rho(t_1) = \frac{1}{N}I$ then $\rho(t_2)$ remains at $\frac{1}{N}I$, substitute them into the Kraus operator sum representation, we will get an extra condition

$$\sum_i K_i K_i^\dagger = I.$$

We will show these two conditions are enough to ensure the dynamics to be majorization monotone. First let's diagonalize $\rho(t_1)$ and $\rho(t_2)$:

$$\begin{aligned}\rho(t_1) &= U_1 \Lambda(\rho(t_1)) U_1^\dagger, \\ \rho(t_2) &= U_2 \Lambda(\rho(t_2)) U_2^\dagger,\end{aligned}$$

where $\Lambda(\rho)$ are diagonal matrix with eigenvalues of ρ as its diagonal entries, substitute them into Eq. (11), we get

$$\begin{aligned}U_2 \Lambda(\rho(t_2)) U_2^\dagger &= \sum_i K_i U_1 \Lambda(\rho(t_1)) U_1^\dagger K_i^\dagger, \\ \Lambda(\rho(t_2)) &= \sum_i U_2^\dagger K_i U_1 \Lambda(\rho(t_1)) U_1^\dagger K_i^\dagger U_2.\end{aligned}\quad (12)$$

Let $V_i = U_2^\dagger K_i U_1$, then

$$\Lambda(\rho(t_2)) = \sum_i V_i \Lambda(\rho(t_1)) V_i^\dagger, \quad (13)$$

and it is easy to check that

$$\begin{aligned}\sum_i V_i V_i^\dagger &= U_2^\dagger \left(\sum_i K_i K_i^\dagger \right) U_2 = I, \\ \sum_i V_i^\dagger V_i &= U_1^\dagger \left(\sum_i K_i K_i^\dagger \right) U_1 = I.\end{aligned}\quad (14)$$

It is a linear map from the eigenvalues of $\rho(t_1)$ to eigenvalues of $\rho(t_2)$, so we can find a matrix D , such that

$$\lambda(\rho(t_2)) = D \lambda(\rho(t_1)), \quad (15)$$

where $\lambda(\rho)$ is a vector in \mathbb{R}^N with eigenvalues of ρ as its entries, which is arranged in the same order as the diagonal entries of $\Lambda(\rho)$. The matrix D can be computed from Eq. (13):

$$D_{\alpha\beta} = \sum_i |(V_i)_{\alpha\beta}|^2,$$

where $D_{\alpha\beta}$ and $(V_i)_{\alpha\beta}$ are the $\alpha\beta$ entry of D and V_i respectively. It is straightforward to show that, by using the two conditions in Eq. (14),

$$\begin{aligned}\sum_\alpha D_{\alpha\beta} &= 1, \\ \sum_\beta D_{\alpha\beta} &= 1,\end{aligned}$$

i.e., D is a doubly stochastic matrix. From Proposition 2, we get

$$\lambda(\rho(t_2)) \prec \lambda(\rho(t_1)),$$

so

$$\rho(t_2) \prec \rho(t_1), \forall t_2 > t_1,$$

i.e. it is majorization monotone.

From Proposition 5 and 6, it is easy to see that majorization monotone implies entropy monotone and trace norm monotone, and they share the same necessary and sufficient condition: $L(I) = 0$.

V. CONCLUSION

Understanding open quantum systems is an important problem for a wide variety of physics, chemistry, and engineering applications. This paper analyzed the dynamics of open quantum systems and gives necessary and sufficient condition on majorization monotone dynamics, which are those dynamics always mixing the states. This suggests that for this class of dynamics, majorization defines an evolution arrow, which begs for the connection to the entropy arrow in the second law of thermal dynamics. I hope further investigation will reveal more on this connection.

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